



Petascale Computing Resource Allocations PRAC – NSF 14-518

Rudi Eigenmann, NSF CISE/ACI
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Join us

The Directorate for Computer and Information Science and Engineering (CISE) is seeking qualified candidates for a Program Director for the High Performance Computing (HPC) program, which is managed in the Division of Advanced Cyberinfrastructure (ACI).

<https://www.usajobs.gov/GetJob/ViewDetails/358941800?org=ACI>

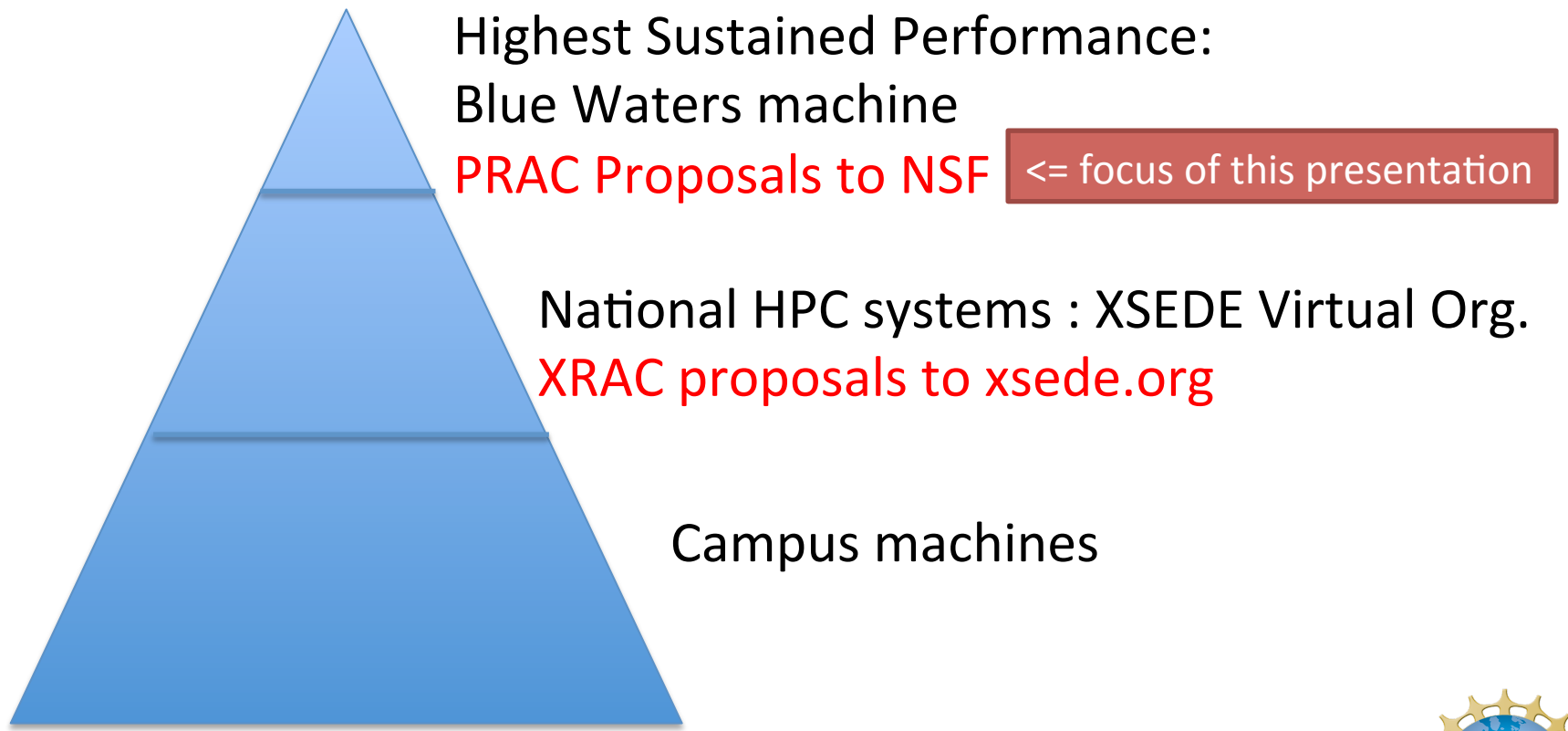


Agenda

- Program description
- FAQs
- Questions and answers



Key Enabler of Science and Engineering: Community Access to Computational Capabilities



FY 14 Solicitation (NSF 14-518)

- Request computing allocations on Blue Waters
- You must demonstrate that
 - You have a breakthrough science or engineering research problem that requires petascale computing capabilities
 - Your code requires and can effectively exploit the capabilities offered by Blue Waters.
- Proposals from or including junior researchers are encouraged
- Next PRAC deadline is March 10, 2014



Type of Award

- Compute allocation
Represents significant investment of NSF
⇒ rigorous, competitive review of both the science and the suitability for execution on Blue Waters
- Consulting expertise from the Blue Waters team
- Up to \$40,000 for travel by your team or the Blue Waters team

10-15 awards anticipated



Goal of Blue Waters, PRAC

- To advance the frontiers of science and engineering by providing a computational capability that makes it possible for investigators to tackle much larger and more complex research challenges across a wide spectrum of domains.

*You will get access to one of the most terrific research tools
“to boldly take science where no-one has taken it before!”*

- To build a community capable of using petascale computing.



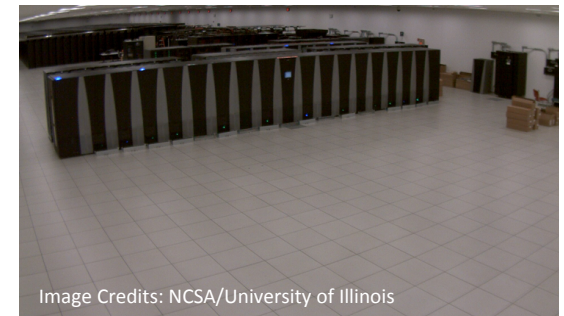
Example Science Domains of Interest

- materials science,
- nano-engineering,
- fluid dynamics,
- climate and earth system dynamics,
- cosmology and astrophysics,
- chemistry and biochemistry,
- sustainability,
- health information technologies,
- cybersecurity,
- economics and social science,
- neuroinformatics and bioinformatics,
- many different topics within physics, engineering, and increasingly in cross-disciplinary sciences.



The Blue Waters Machine

- Petascale system – sustained performance above 1 petaflop/s
- Deployed at the University of Illinois
- Tackle much larger and more complex research challenges than in the past, across a wide spectrum of domains
- Achieve significant impacts by
 - creating new knowledge about the natural world
 - increasing industrial competitiveness
 - improving national security
- Blue Waters entered full-scale operation in 2013



Blue Waters Architecture

Designed for sustained petascale performance on several 100,000 cores for a broad class of problems

- 22,640 XE6 compute nodes @ 16 AMD cores = 362,240 cores
- 4,224 XK compute nodes @ 8 cores + 1 NVIDIA Kepler GPU
- 7.1 + 6.24 PF peak performance
- 1.382 PB + 135 TB memory
- I/O system: >1TB/s bandwidth, 26.4 PB
- High-speed interconnect: 3D Torus, Cray Gemini
- Supports visualization of large datasets produced by computations
- More info: bluewaters.ncsa.illinois.edu/hardware-summary



Performance Optimization

Optimizing your code on Blue Waters may entail:

- Discovering and exploiting parallelism within codes
- Overlapping different types of operations
- Exploiting multi-level caches, local/remote memory
- Orchestrating intra/inter-node communication
- Performing parallel I/O
- Exploiting heterogeneous processors
- Dealing with petabyte-size memory-resident data and correspondingly large input-output datasets

You need to show you have the necessary expertise



Development Plan

Several years of preparation may be needed to get ready to exploit a sustained petaflop system.

Present a development plan, such as:

- Code scalability today
- Year 1: Optimizations for scalability to part of machine
- Year 2: Further optimizations for full scalability

The Blue Waters team will provide consultation and support. Indicate in the plan tasks for which you need help

bluewaters.ncsa.illinois.edu/contact-us



Project Description

- Target research problem
- Intellectual merit
- Broader impact
- Description of computational code(s)
- Development plan and source of funding
- Computational resources required
 - Number and type of compute nodes
 - Memory usage
 - Number and duration of runs for each development phase
 - Total number of node hours, I/O requirements

Disclose resources allocated or proposed from other sources



Review Criteria

- Intellectual Merit and Broader Impact
- Is the proposed research leading to breakthrough science and engineering?
- Does it require the capability of a resource such as Blue Waters?



FAQ 1

- Q: How can I tell if my proposed work is a good fit for the PRAC program?
- A: A successful PRAC proposal shows that
 - You have a very important science or engineering research problem that requires petascale computing capabilities
 - You have a solid plan to effectively exploit the massive capabilities offered by the Blue Waters machine



FAQ 2

- Q: Can I be PI on one proposal and co-PI on another?
- A: No, but you may be listed as senior personnel on another PRAC proposal



FAQ 3

- Q: Should I discuss my proposal with NSF Program Directors?
- A: Yes, PIs are welcome to discuss planned proposals with the Program Director. When you call, good knowledge of the solicitation will be appreciated.
Once submitted, the substance of proposals will not be discussed by NSF Program Directors, as this would constitute unfair competition, or the perception thereof.



FAQ 4

- Q: If PRAC does not fund the development of the computational application, who does?
- A: You will need to write a proposal to an NSF directorate or another agency that sponsors research in your science domain. Once you get it funded, consider writing a PRAC proposal.



FAQ 5

- Q: Would it be better for me to write an XRAC proposal and send it to xsede.org?
- A: Getting an XSEDE allocation is better if
 - You are only beginning to parallelize your code.
Request a startup allocation
 - You don't have funding for developing your application into an efficient parallel code
 - Your code scales well, but does not need the massive capabilities of Blue Waters



FAQ 6

- Q: Will there be future PRAC deadlines?
- A: Yes, the deadlines are:

March 10, 2014

November 14, 2014

November 13, 2015

November 09, 2016





Petascale Computing Resource Allocations (PRAC)

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